

10/561,949

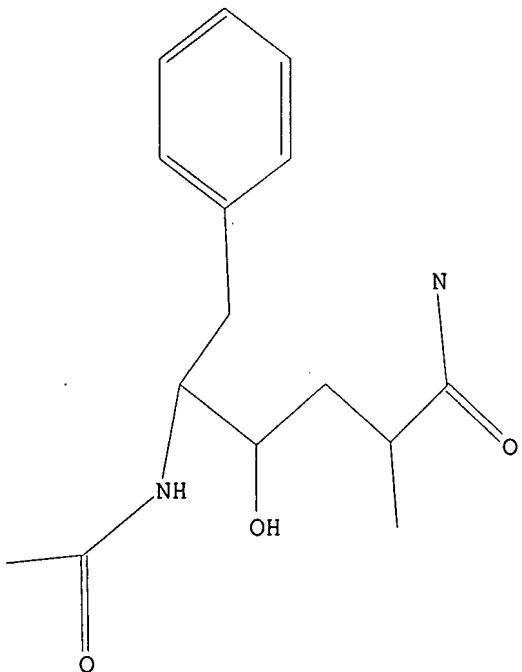
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exact/norm bonds :
1-7 7-8 8-9 9-18 10-11 15-16 15-17 18-19 18-20
exact bonds :
8-10 10-12 12-13 13-14 13-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS

L10 STRUCTURE UPLOADED

=> dis
L10 HAS NO ANSWERS
L10 STR



G1 C,O,N

Structure attributes must be viewed using STN Express query preparation.

=> s L10 full

10/561,949

FULL SEARCH INITIATED 13:17:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4078 TO ITERATE

100.0% PROCESSED 4078 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

L11 15 SEA SSS FUL L10

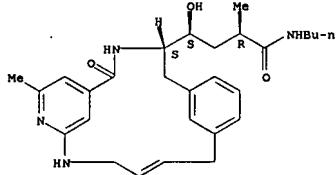
=> fil hcap uspatful
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
863.20 863.41

FILE 'HCAPLUS' ENTERED AT 13:17:56 ON 02 MAY 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE 'USPATFULL' ENTERED AT 13:17:56 ON 02 MAY 2007
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> L11
L12 3 L11

=> d L12 1-3 ibib abs hitstr

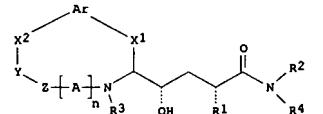


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 3 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:29320 HCPLUS
 DOCUMENT NUMBER: 142:134632
 TITLE: Macrocyclic compounds having aspartic protease inhibiting activity and pharmaceutical uses thereof
 INVENTOR(S): Betschart, Claudia; Tintelnot-Bloemley, Marina
 PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
 SOURCE: PCT Int. Appl., 38 pp.
 CODEN: PIXKD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 20050113	A1	WO 2004-EP7247	20040702	
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MW, NA, SD, SL, SZ, TZ, WG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004253667	A1	AU 2004-253667	20040702	
CA 2529571	A1	CA 2004-2529571	20040702	
EP 1654241	A1	EP 2004-740596	20040702	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1809542	A	CN 2004-80017405	20040702	
BR 2004012286	A	BR 2004-12286	20040702	
US 2006223745	A1	US 2005-561949	20051222	
PRIORITY APPLN. INFO.: US 2003-15654		GB 2003-15654		A 20030703
		WO 2004-EP7247		W 20040702

OTHER SOURCE(S): MARPAT 142:134632
 GI



AB The preparation of macrocyclic compds., I, (R1 = alkyl, alkoxy, piperidinyl,

L12 ANSWER 2 OF 3 HCPLUS COPYRIGHT 2007 ACS on STN (Continued)
 or pyrrolidinyl; R2, R4 = H, alkyl, cycloalkyl, aryl, heteroaryl etc or R2 and R4, together with the nitrogen to which they are attached, form an optionally substituted piperidino, pyrrolidinyl, morpholino or piperazinyl

group; R3 = H, alkyl; X1 = CH2; X2 = CH2, O, S, COO, OCO, NHCO, CONH, or NR, R being hydrogen or (C1-4)alkyl; Y (C1-8)alkylen or (C1-8)alkylenoxy(C1-6)alkylen, (C1-8)alkylen or (C1-8)alkylenoxy(C1-6)alkylen; Ar = a Ph ring optionally mono- di- or trisubstituted; Z = CO, A = a natural or unnatural alpha-amino-acid; and n is 0 or 1, or Z = S(=O)2 and AA = an optionally substituted ethylenecarbonyl group (derived from a natural or unnatural alpha-amino acid by replacement of the nitrogen by a methylene group), and n is 1) are prep'd. as aspartic protease inhibitors for the treatment of neurol. and vascular disorders related to beta-amyloid generation and/or aggregation.

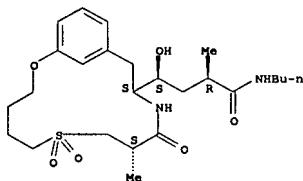
IT 824429-16-3P 824429-24-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (macrocyclic compds. having aspartic protease inhibiting activity and pharmaceutical uses thereof)

RN 824429-16-3 HCPLUS

CN 2-Oxa-7-thia-11-azabicyclo[12.3.1]octadeca-1(18),14,16-triene-12-butanoate, N-butyl-γ-hydroxy-α,9-dimethyl-10-oxo-, 7,7-dioxide, (αR,γS,9S,12S)- (9CI) (CA INDEX NAME)

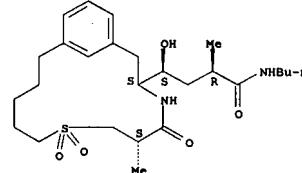
Relative stereochemistry.



RN 824429-24-5 HCPLUS
 CN 8-Thia-4-azabicyclo[12.3.1]octadeca-1(18),14,16-triene-3-butanamide, N-butyl-γ-hydroxy-α,6-dimethyl-3-oxo-, 8,8-dioxide, (αR,γS,3S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 2 OF 3 HCPLUS COPYRIGHT 2007 ACS on STN (Continued)



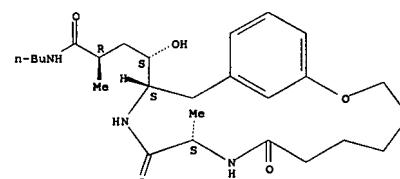
IT 824429-11-OP 824429-29-OP 824957-23-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (macrocyclic compds. having aspartic protease inhibiting activity and pharmaceutical uses thereof)

RN 824429-11-0 HCPLUS

CN 2-Oxa-9,12-diazabicyclo[13.3.1]nonadeca-1(19),15,17-triene-13-butanamide, N-butyl-γ-hydroxy-α,10-dimethyl-8,11-dioxo-, (αR,γS,10S,13S)- (9CI) (CA INDEX NAME)

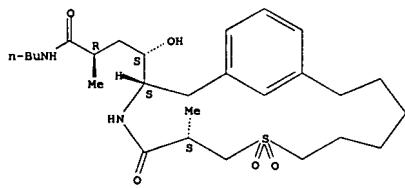
Absolute stereochemistry.



RN 824429-29-0 HCPLUS

CN 8-Thia-4-azabicyclo[13.3.1]nonadeca-1(19),15,17-triene-3-butanamide, N-butyl-γ-hydroxy-α,6-dimethyl-5-oxo-, 8,8-dioxide, (αR,γS,3S,6S)- (9CI) (CA INDEX NAME)

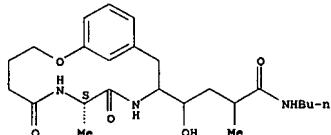
Absolute stereochemistry.



RN 824957-23-5 HCPLUS

CN 2-Oxa-7,10-diazabicyclo[11.3.1]heptadeca-1(17),13,15-triene-11-butanamide, N-butyl-γ-hydroxy-α,8-dimethyl-6,9-dioxo-, (8S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



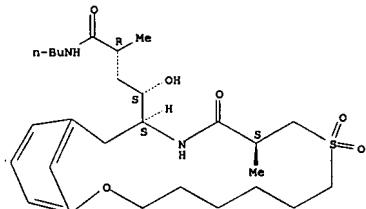
IT 824429-15-4P 824429-21-2P 824429-23-4P

824957-22-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(macrocyclic compds. having aspartic protease inhibiting activity and pharmaceutical uses thereof)

RN 824429-15-4 HCPLUS

CN 2-Oxa-9-thia-13-azabicyclo[14.3.1]eicosa-1(20),16,18-triene-14-butanamide, N-butyl-γ-hydroxy-α,11-dimethyl-12-oxo-, 9,9-dioxide, (αR,γS,11S,14S)-rel- (9CI) (CA INDEX NAME)

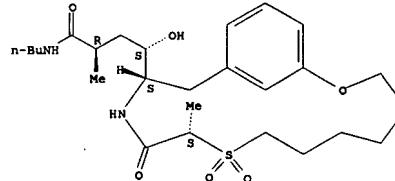
Relative stereochemistry.



RN 824429-21-2 HCPLUS

CN 2-Oxa-9-thia-12-azabicyclo[13.3.1]nonadeca-1(19),15,17-triene-13-butanamide, N-butyl-γ-hydroxy-α,10-dimethyl-11-oxo-, 9,9-dioxide, (αR,γS,10S,13S)- (9CI) (CA INDEX NAME)

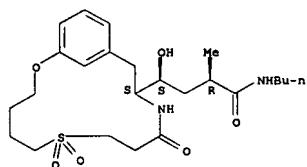
Absolute stereochemistry.



RN 824429-23-4 HCPLUS

CN 2-Oxa-7-thia-11-azabicyclo[12.3.1]octadeca-1(18),14,16-triene-12-butanamide, N-butyl-γ-hydroxy-α-methyl-10-oxo-, 7,7-dioxide, (αR,γS,12S)-rel- (9CI) (CA INDEX NAME)

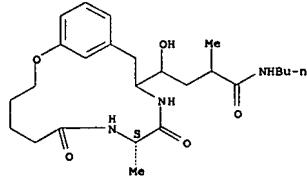
Relative stereochemistry.



RN 824957-22-4 HCPLUS

CN 2-Oxa-8,11-diazabicyclo[12.3.1]octadeca-1(18),14,16-triene-12-butanamide, N-butyl-γ-hydroxy-α,9-dimethyl-7,10-dioxo-, (9S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 3 USPATFULL on STN
ACCESSION NUMBER: 2006-262229 USPATFULL
TITLE: Macrocyclic compounds having aspartic protease inhibiting activity and pharmaceutical uses thereof
INVENTOR(S): Betschart, Claudia, Basel, SWITZERLAND
Tintelnot-Bloniley, Marina, Maulburg, GERMANY, FEDERAL REPUBLIC OF

NUMBER	KIND	DATE
US 2006223745	A1	20061005
US 2004-561949	A1	20040702 (10)
WO 2004-EP7247		20040702 20051222 PCT 371 date

NUMBER	DATE
GB 2003-15654	20030703

PRIORITY INFORMATION: GB 2003-15654 20030703
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: NOVARTIS, CORPORATE INTELLECTUAL PROPERTY, ONE HEALTH PLAZA 104/3, EAST HANOVER, NJ, 07936-1080, US
NUMBER OF CLAIMS: 12
EXEMPLARY CLAIM: 1
LINE COUNT: 1191
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention relates to macrocyclic compounds of formula (I), wherein R. sub.1, is (C. sub.1-8)alkyl, (C. sub.3-7)alkoxy(C. sub.1-4)alkyl, hydroxy(C. sub.1-6)alkyl, (C. sub.1-4)alkylthio(C. sub.1-4)alkyl, (C. sub.3-7)cycloalkyl(C. sub.1-4)alkyl, (C. sub.1-4)alkyl, piperidinyl or pyrrolidinyl, R. sub.2 and R. sub.4, independently, are hydrogen or optionally substituted (C. sub.1-8)alkyl, (C. sub.3-7)cycloalkyl, (C. sub.1-4)alkyl, heteroaryl or heteroaryl(C. sub.1-4)alkyl, or R. sub.2 and R. sub.4, together with the nitrogen to which they are attached, form an optionally substituted piperidino, pyrrolidinyl, morpholino or piperazinyl group, R. sub.3 is hydrogen or (C. sub.1-4)alkyl, X. sub.1 is CH. sub.2, X. sub.2 is CH. sub.2, O, S, CO, COO, OCO, NHCO, CONH, or NR, R being hydrogen or (C. sub.1-4)alkyl, Y is (C. sub.1-8)alkenyl or (C. sub.1-8)alkylenoxy(C. sub.1-6)alkenyl, (C. sub.1-8)alkenyl or (C. sub.1-6)alkylenoxy(C. sub.1-6)alkenyl, At is a phenyl ring optionally mono- di or tri-substituted by, independently, hydroxy or halogen, whereby X. sub.1, and X. sub.2 are in meta or para position to each other, and either Z is CO, AA is a natural or unnatural alpha-amino-acid, and n is 0 or 1, or Z is SO. sub.2, AA is an optionally substituted ethylenecarbonyl group (derived from a natural or unnatural alpha-amino-acid by replacement of the nitrogen by methylene group), and n is 1; processes for the preparation of these compounds, pharmaceutical compositions and combinations comprising the same; and their use in the treatment of neurological and vascular disorders related to beta-amyloid generation and/or aggregation. ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 824429-16-5P 824429-24-5P
(macrocyclic compds. having aspartic protease inhibiting activity and

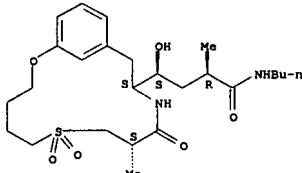
L12 ANSWER 3 OF 3 USPATFULL on STN (Continued)

pharmaceutical uses thereof)

RN 824429-16-5 USPATFULL

CN 2-Oxa-7-thia-11-azabicyclo[12.3.1]octadeca-1(18),14,16-triene-12-butanamide, N-butyl- γ -hydroxy- α ,9-dimethyl-10-oxo-, 7,7-dioxide, (aR, γ S, 9S, 12S)-rel- (9CI) (CA INDEX NAME)

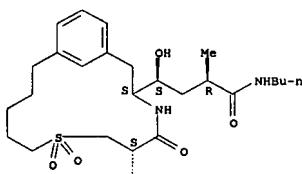
Relative stereochemistry.



RN 824429-24-5 USPATFULL

CN 8-Thia-4-azabicyclo[12.3.1]octadeca-1(18),14,16-triene-3-butanamide, N-butyl- γ -hydroxy- α ,6-dimethyl-5-oxo-, 8,8-dioxide, (aR, γ S, 3S, 6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

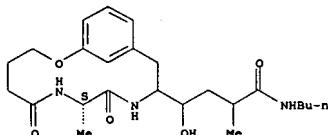
IT 824429-11-0P 824429-29-0P 824957-23-5P
(macrocyclic compds. having aspartic protease inhibiting activity and pharmaceutical uses thereof)

RN 824429-11-0 USPATFULL

CN 2-Oxa-9,12-diazabicyclo[13.3.1]nonadeca-1(19),15,17-triene-13-butanamide, N-butyl- γ -hydroxy- α ,10-dimethyl-8,11-dioxo-, (aR, γ S, 10S, 13S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

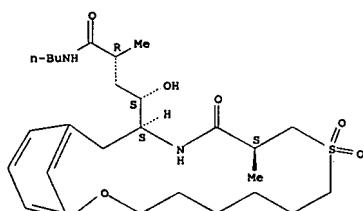
L12 ANSWER 3 OF 3 USPATFULL on STN (Continued)

IT 824429-15-4P 824429-21-2P 824429-23-4P
824957-22-4P
(macrocyclic compds. having aspartic protease inhibiting activity and pharmaceutical uses thereof)

RN 824429-15-4 USPATFULL

CN 2-Oxa-9-thia-13-azabicyclo[14.3.1]eicosa-1(20),16,18-triene-14-butanamide, N-butyl- γ -hydroxy- α ,11-dimethyl-12-oxo-, 9,9-dioxide, (aR, γ S, 11S, 14S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 824429-21-2 USPATFULL

CN 2-Oxa-9-thia-12-azabicyclo[13.3.1]nonadeca-1(19),15,17-triene-13-butanamide, N-butyl- γ -hydroxy- α ,10-dimethyl-11-oxo-, 9,9-dioxide, (aR, γ S, 10S, 13S)- (9CI) (CA INDEX NAME)

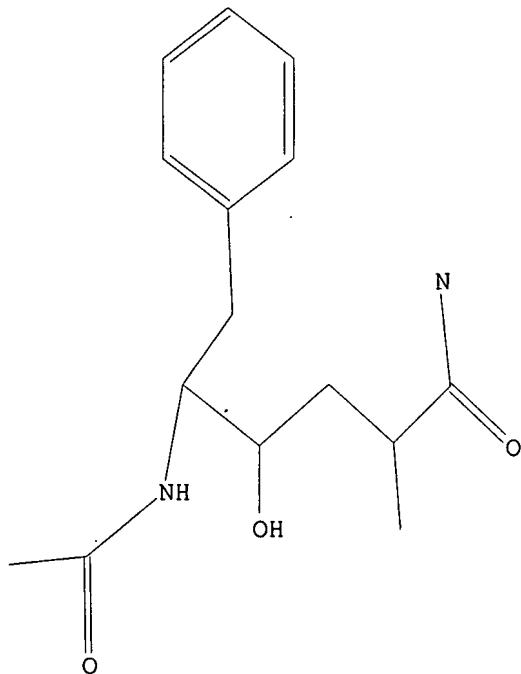
Absolute stereochemistry.

10/561,949

L12 ANSWER 3 OF 3 USPATFULL on STN (Continued)

10/561,949

=> d que stat
L10 STR



G1 C, O, N

Structure attributes must be viewed using STN Express query preparation.

L11 15 SEA FILE=REGISTRY SSS FUL L10
L12 3 SEA L11

=> d his full

(FILE 'HOME' ENTERED AT 13:10:49 ON 02 MAY 2007)

FILE 'REGISTRY' ENTERED AT 13:11:03 ON 02 MAY 2007

L1 STRUCTURE UPLOADED
DIS
L2 0 SEA SSS SAM L1
L3 0 SEA SSS FUL L1
L4 STRUCTURE UPLOADED
DIS
L5 0 SEA SSS FUL L4
L6 STRUCTURE UPLOADED
DIS
L7 0 SEA SSS FUL L6
L8 STRUCTURE UPLOADED
DIS
L9 0 SEA SSS FUL L8
L10 STRUCTURE UPLOADED
DIS
L11 15 SEA SSS FUL L10

10/561,949

FILE 'HCAPLUS, USPATFULL' ENTERED AT 13:17:56 ON 02 MAY 2007
L12 3 SEA ABB=ON PLU=ON L11
D L12 1-3 IBIB ABS HITSTR
D QUE STAT

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8
DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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<http://www.cas.org/support/stngen/stndoc/properties.html>

FILE HCAPLUS

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FILE COVERS 1907 - 2 May 2007 VOL 146 ISS 19
FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 1 May 2007 (20070501/PD)
FILE LAST UPDATED: 1 May 2007 (20070501/ED)
HIGHEST GRANTED PATENT NUMBER: US7213269
HIGHEST APPLICATION PUBLICATION NUMBER: US2007094759
CA INDEXING IS CURRENT THROUGH 1 May 2007 (20070501/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 1 May 2007 (20070501/PD)

10/561,949

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2006
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2006

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---Logging off of STN---

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Executing the logoff script...

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FULL ESTIMATED COST	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
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STN INTERNATIONAL LOGOFF AT 13:19:45 ON 02 MAY 2007